

Benzoic acid, 2-nitro-, methyl ester

Other names:	Benzoic acid, o-nitro-, methyl ester Methyl 2-nitrobenzoate Methyl o-nitrobenzoate Methyl ortho-nitrobenzoate
Inchi:	InChI=1S/C8H7NO4/c1-13-8(10)6-4-2-3-5-7(6)9(11)12/h2-5H,1H3
InchiKey:	AOXPHVNMBPFOFS-UHFFFAOYSA-N
Formula:	C8H7NO4
SMILES:	COC(=O)c1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	181.15
CAS:	606-27-9

Physical Properties

Property code	Value	Unit	Source
gf	-79.11	kJ/mol	Joback Method
hf	-238.95	kJ/mol	Joback Method
hfus	24.28	kJ/mol	Joback Method
hvap	62.09	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	1.381		Crippen Method
mcvol	124.680	ml/mol	McGowan Method
pc	3848.31	kPa	Joback Method
tb	548.20	K	NIST Webbook
tc	889.97	K	Joback Method
tf	434.63	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.26	J/mol×K	642.23	Joback Method
cpg	308.88	J/mol×K	683.52	Joback Method
cpg	318.68	J/mol×K	724.81	Joback Method
cpg	327.67	J/mol×K	766.10	Joback Method
cpg	335.88	J/mol×K	807.39	Joback Method

cpg	343.31	J/mol×K	848.68	Joback Method
cpg	349.99	J/mol×K	889.97	Joback Method
hvapt	56.10	kJ/mol	438.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.83733e+01
Coeff. B	-9.61945e+03
Coeff. C	1.11957e+02
Temperature range (K), min.	419.93
Temperature range (K), max.	624.50

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C606279&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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